



>>Entry Name: 2-Amino-3-(4-nitrophenyl)propanoic acid

Synonym(s): 3-(4-Nitrophenyl)alanine, 9Cl. α -Amino-4-nitrobenzenepropanoic acid

CAS Registry Number: 1991-83-9

Related CAS Registry Numbers(s): 56613-61-7 120108-64-7 147065-06-3

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 949-99-5

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 239-241 dec.°

Optical Rotation: $[\alpha]_D^{27} +9.4$ (c, 1 in 1M HCl)

Fluka: 73615

Sigma: N0884

>>Derivative: Me ester

Molecular Formula: $C_{10}H_{12}N_2O_4$

Molecular Weight: 224.216

Accurate Mass: 224.079708

Percentage Composition: C 53.57%; H 5.39%; N 12.49%; O 28.54%

Physical Description: Needles (EtOH) (as hydrochloride)

Melting Point: Mp 227-228° (hydrochloride)

>>Derivative: *N*-tert-Butyloxycarbonyl

CAS Registry Number: 33305-77-0

Molecular Formula: $C_{14}H_{18}N_2O_6$

Molecular Weight: 310.306

Accurate Mass: 310.116488

Percentage Composition: C 54.19%; H 5.85%; N 9.03%; O 30.94%

Physical Description: Cryst. (diisopropyl ether/hexane)

Melting Point: Mp 107°

Optical Rotation: $[\alpha]_{578}^{25} +7.94$ (c, 1.55 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 2922-40-9

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

Physical Description: Cryst.

Melting Point: Mp 242-243 dec.°

Sigma: N9501

>>Derivative: Hydrochloride

CAS Registry Number: 66693-69-4

Physical Description: Cryst.

Melting Point: Mp 230°

References: